Geometric phase in external electromagnetic fields

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Variations of *polarization* is a dielectric property of quantum systems, quantified by Resta et al. [1], and discovered to be a Berry phase[2] of the electronic subsystem. In order to continue the previous research we wrote a scalar phase Φ as the *circulation* of the polarization field, a vector field called *dipole moment per unit volume* $\bar{P}$, or in alternative and in a more general form as the flux of a *new* vector field called *macroscopic rotonic field* indicated with $\mathbf{L}^+$. The latter shows to be a more general berry phase concerning the interaction of the electronic subsystem with an external electromagnetic field.

INTRODUCTION

In this paper is developed a model in order to introduce a general definition of a Berry phase[3, 4] concerning the interaction of the electronic subsystem with a uniform static electromagnetic field. The latter phase is what I call a scalar quantum phase, a Berry phase. This heuristic study is based on mechanical and electrical properties of the electronic field in its steady states[5]. Firstly, we introduce several equations useful for the derivation of the scalar phase when only a uniform electrostatic field is interacting with the electronic field, we then generalize the result considering also an external magnetic field interacting with the electronic subsystem. A derivation of two *new* vectorial fields will be given and their relation to geometric phases will be exploited.

GROUP VELOCITY IN FINITE ELECTROSTATIC FIELDS

In this section we derive heuristically or better theoretically the expression of the *group velocity* of the electronic field as a first step of our understanding of the dielectric responce of the latter when it is interacting with an external electrostatic field. We make use of a particular *gauge representation*, the $k - q$ representation[6]. We always considered the eigenstates of the system as follows:

$$\Psi_{n,\mathbf{k}} = e^{i\mathbf{k}\cdot\mathbf{q}} u_{n,\mathbf{k}} \tag{1}$$

and the system being in its steady states[5]. The Hamiltonian is written as follows:

$$H_{\mathbf{k}} \equiv [\frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k})^2 - \mathbf{E^0}\cdot i\nabla_{\mathbf{k}} + V(\mathbf{q})] \tag{2}$$

where $\mathbf{E^0}$ is a uniform static external electric field.

It is already known that the expectation values of the *group velocity* operator[5]:

$$\hat{\mathbf{v}} = \frac{1}{m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k}) \tag{3}$$

in a vanishing external electromagnetic field are written as follows:

$$\mathbf{v_{mn}} = < u_{m,\mathbf{k}}|\hat{\mathbf{v}}|u_{n,\mathbf{k}} > \tag{4}$$

The same result holds when a uniform static electric field is present in the system by direct application of theorem in[5] to the Hamiltonian (2). In absence of external fields it has been shown[3] that:

$$\mathbf{v_{mn}} = -i\omega_{\mathbf{mn}}\mathbf{d_{mn}} + \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon_{n,\mathbf{k}}\delta_{\mathbf{mn}} \tag{5}$$

previous result *holds* also for any applied external uniform electrostatic field present in the system. Transition frequencies are written as: $\omega_{\mathbf{mn}} = \frac{\epsilon_{m,\mathbf{k}}-\epsilon_{n,\mathbf{k}}}{\hbar}$ and $\mathbf{v_{mn}}$ are matrix elements. Matrix elements $\mathbf{d_{mn}}$ are instead the matrix elements of the *position* operator, and are defined as:

$$\mathbf{d_{mn}} = < u_{m,\mathbf{k}}|i\nabla_{\mathbf{k}}|u_{n,\mathbf{k}} > \tag{6}$$

and because of the normalization condition on the amplitudes $u_{n,\mathbf{k}}$ follows that:

$$\mathbf{d_{mn}^*} = \mathbf{d_{nm}} \tag{7}$$

implying that diagonal fields $\mathbf{d_{nn}}$ are real, and the matrix $\mathbf{d_{nm}}$ is Hermitian. It is possible to show to be valid the following relations:

$$\mathbf{d_{mn}} = i\frac{\mathbf{v_{mn}}}{\omega_{\mathbf{mn}}} \quad m \neq n$$
$$\mathbf{v_{nn}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon_{n,\mathbf{k}} \quad m = n \tag{8}$$

as previously shown by[3] when vanishing external fields are concerned. It is remarkable that the second definition, of eq.(8), can be directly derived by the theorem stated in[5]. It represents the *group velocity*[5] of the electronic subsystem. Armed with the previous result we derive[3] a Berry phase of the electronic system in the following section.

SCALAR PHASE IN ETERNAL ELECTROSTATIC FIELDS

Here we derive a Berry phase of the electronic field bearing in mind that the Hamiltonian of the system is reported in eq.(2). As shown by Zak and Berry[2, 4], we can write:

$$\int_S d\mathbf{S} \cdot \mathbf{Im} \sum_{m \neq n} [\frac{\mathbf{v_{mn}} \times \mathbf{v_{nm}}}{\omega_{mn}^2}] = \int_S d\mathbf{S} \cdot \nabla_{\mathbf{k}} \times \mathbf{d_{nn}} \quad (9)$$

where S is a closed surface of the system, Brillouine zone, and C is a curve contained in that surface. Also,

$$\int_S d\mathbf{S} \cdot \nabla_{\mathbf{k}} \times \mathbf{d_{nn}} = \oint_C \mathbf{d_{nn}} \cdot d\mathbf{l} \quad (10)$$

and finally,

$$\oint_C \mathbf{d_{nn}} \cdot d\mathbf{l} = \phi_n \quad (11)$$

On the other hand, we can write[2, 4]:

$$\int_S d\mathbf{S} \cdot \mathbf{Im} \sum_{\mathbf{m \neq n}} \mathbf{d_{mn}} \times \mathbf{d_{nm}} = \int_{\mathbf{S}} d\mathbf{S} \cdot \nabla_{\mathbf{k}} \times \mathbf{d_{nn}} \quad (12)$$

It is then possible to express ϕ_n in another way:

$$\int_S d\mathbf{S} \cdot \mathbf{Im} \sum_{\mathbf{m \neq n}} \mathbf{d_{mn}} \times \mathbf{d_{nm}} = \phi_{\mathbf{n}} \quad (13)$$

where **Im** stands for imaginary.

After a summation over n, it is possible to evaluate:

$$\sum_n \phi_n = \Phi \quad (14)$$

where Φ is a *conserved geometric phase* (a Berry phase). We shall call Φ a first scalar phase[2]. The averaged trace of fields $\mathbf{d_{mn}}$ can be calculated by integration over the Brillouin zone in reciprocal space as and gives the macroscopic polarization[1, 7]:

$$\bar{\mathbf{P}} = \frac{e}{(2\pi)^3} \int_{BZ} dk \mathbf{Tr}(\mathbf{d_{mn}}) \quad (15)$$

It is possible to define a *dipolar field* as follows:

$$\mathbf{P} = e\mathbf{Tr}(\mathbf{d_{mn}}) \quad (16)$$

Making use of equations (11)(14)(16)allows us to define the scalar phase as follows:

$$\oint_C \mathbf{P} \cdot d\mathbf{l} = e\Phi \quad (17)$$

where C is a closed curve contained in the surface of the Brillouin zone. Berry phase instead is given by eq.(17) and quantifies the amount of polarization charge $e\Phi$ *stored* on the surface of the system (a unit cell if the system is a crystal[8]). We may calculate the conserved phase Φ, not only by the knowledge of matrix elements of the velocity operators, as in eq.(9),(10),(11), but also by the knowledge of matrix elements $\mathbf{d_{mn}}$ eq.(13). Result of eq.(17) is also in agreement with the modern theory of polarisation where the phase Φ is proportional to the Chern number of a Chern-insulator[9, 10], we still consider it either a Berry or a Zak phase calling it a scalar geometric phase. In the following, we extend the problem to find a scalar phase proportional to the Chern number to the case of an external uniform magnetostatic field interacting with the electronic field.

SCALAR PHASE IN ELECTROMAGNETIC FIELDS

In this section we generalize the problem to the case of also an external uniform magnetostatic field B^0 interacting with the electronic system.

We can write the Hamiltonian of the system[6] as follows:

$$H_{\mathbf{k}} \equiv [\frac{1}{2m}(-i\hbar\nabla_{\mathbf{q}} + \hbar\mathbf{k} - \frac{e}{2c}B^0 \times i\nabla_{\mathbf{k}})^2 - E_0 \cdot i\nabla_{\mathbf{k}} + V(\mathbf{q})] \quad (18)$$

where e is the elementary electronic charge.

In analogy to eq. (4) we can define the following matrix:

$$\mathbf{v^{(B^0)}}_{mn} = -i\omega_{\mathbf{mn}}\mathbf{d_{mn}} + \mathbf{V_{mn}} + \frac{e}{2mc}B^0 \times \mathbf{d_{mn}} \quad (19)$$

where,

$$\mathbf{V_{mn}} = \frac{1}{\hbar} \nabla_{\mathbf{k}} \epsilon_n \delta_{\mathbf{mn}} \qquad (20)$$

We shall see that the scalar phase introduced in eq.(17) can be directly obtained as the *flux* over a closed surface of a new vectorial field. Let us define:

$$\mathbf{l_n^+} = \frac{1}{2} \sum_{m \neq n} \frac{[\mathbf{d_{nm}} \times \mathbf{v_{mn}^{(B^0)}}] + [\mathbf{d_{mn}} \times \mathbf{v_{nm}^{(B^0)}}]}{\omega_{mn}}$$
$$= \mathbf{rot\ d_{nn}} \qquad (21)$$

where $\mathbf{rot\ d_{nn}} = \nabla_k \times \mathbf{d_{nn}}$, so that integrating over the surface of the Brillouin zone we obtain:

$$\sum_n \int_{BZ} d\mathbf{S} \cdot \mathbf{rot d_{nn}} = \sum_{\mathbf{n}} \int_{\mathbf{BZ}} d\mathbf{S} \cdot \mathbf{l_n^+} \qquad (22)$$

It is worth noticing here that the vectorial field $\mathbf{l_n^+}$ relates the matrix elements of the velocity operator to the matrix elements of the position operator of the electronic field. Note also that the sum in eq.(21) is weighted by the factors $\frac{1}{\omega_{mn}}$. We can then define a new macroscopic vectorial field as follows:

$$\mathbf{L^+} = \sum_n \mathbf{l_n^+} \qquad (23)$$

and call it *rotonic field*. Also, in analogy to eq.(12),(13),(14) we can define a Berry phase as follows:

$$\Phi^{B^0} = \int_{BZ} d\mathbf{S} \cdot \mathbf{L^+} \qquad (24)$$

expressible as the flux of the rotonic field.

It is clear that eq.(24) is the more general expression of the Berry phase Φ. In fact, in absence of magnetic field the latter expression (24) reduces to eq.(9) once we substitute matrics elements $\mathbf{d_{mn}}$ of eq.(8) in eq.(21).

SUMMARY

A Berry phase Φ, directly dependent on the dielectric properties of the electronic subsystem because of its relation with the polarization field can be expressed, in a purely mechanical way, as the **flux** of the *rotonic field*, $\mathbf{L^+}$, over a closed surface in the Brillouin zone allowing for the definition of the Chern number of the electronic field interacting with an external finite static electromagnetic field.

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